



ELSEVIER

Journal of Magnetism and Magnetic Materials 182 (1998) 341–349

Journal of
Mmagnetism
and
Mmagnetic
materials

Dzyaloshinsky–Moriya interactions induced by symmetry breaking at a surface

A. Crépieux, C. Lacroix*

Laboratoire de Magnétisme Louis Néel, CNRS, BP 166, 38042 Grenoble Cedex 9, France

Received 22 January 1997; received in revised form 25 July 1997

Abstract

We show that antisymmetric exchange interactions $\mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$ occur near magnetic surfaces due to surface symmetry breaking. The direction of the $\mathbf{D}_{ij}$ vectors is determined for several simple surfaces. Consequences of these interactions on magnetic structures are investigated: rearrangement of the magnetic structure close to the surface may occur and non-collinear magnetic structures may be stabilized in thin films. These interactions also contribute to the surface anisotropy. © 1998 Elsevier Science B.V. All rights reserved.

PACS: 7530.Et; 7570.Ak; 7530.Pd

Keywords: Surface magnetism; Exchange interactions – antisymmetric

1. Introduction

Almost 40 years ago, Dzyaloshinsky pointed out, using symmetry arguments, that the combination of low symmetry and spin–orbit coupling gives rise to antisymmetric exchange interactions (AEI) which can be expressed as: $\mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j)$ [1,2]. Moriya has shown how to calculate this AEI for localized magnetic systems in a microscopic model [3,4]: this interaction can be derived by taking into account the spin–orbit coupling in the theory of superexchange interaction proposed by Anderson

[5]. As this interaction vanishes if there is a center of inversion between sites i and j , it is expected to be relevant only when the local symmetry is sufficiently low. The weak ferromagnetism observed in several antiferromagnetic insulating compounds, such as α -Fe₂O₃ or CrF₃, was attributed by Moriya and Dzyaloshinsky to this AEI. More recently it has been proposed that the same interaction is present in the low temperature distorted phases of the La₂CuO₄ and YBa₂Cu₃O₆ type perovskite compounds [6–10].

In the presence of disorder the AEI is also expected to play a role since local symmetry is broken by disorder. The importance of the AEI in spin glass systems was emphasized by several authors [11,12]: it was shown that the AEI leads to

* Corresponding author: Tel.: +33 4 76 88 10 98; fax: +33 4 76 88 11 91; e-mail: lacroix@labs.polycnrs-gre.fr.

remarkably large anisotropy energies in disordered magnetic systems containing nonmagnetic impurities with strong spin–orbit coupling. Fert and Levy in Ref. [12] proposed a different mechanism for AEI which involves both magnetic and non-magnetic sites.

In this paper we show that AEI may also be present close to the surface of a magnetic material, because the symmetry is broken by the surface. This idea was already proposed by Fert in Ref. [13]. Here we calculate the AEI between a surface and a bulk site using Moriya's formalism in a particular case (Section 2.1); we also show that the mechanism proposed by Fert in Ref. [13] leads mainly to AEI between surface sites (Section 2.2); then for any surface, we show that the direction of $\mathbf{D}_{ij}$ can be derived from the symmetry arguments developed by Dzyaloshinsky [1,2]. Finally, in Sections 3 and 4, we show using several examples that the magnetic order can be modified by this interaction in the vicinity of the surface.

2. Derivation of the antisymmetric exchange interaction near a surface

In this section, we calculate the $\mathbf{D}_{ij}$ vector for two different surfaces, using the mechanism proposed either by Moriya (Section 2.1) or by Fert and Levy (Section 2.2); then we derive the direction of $\mathbf{D}_{ij}$ using the symmetry rules for several surfaces (Section 2.3).

2.1. Application of Moriya's formalism to the (0 0 1) surface of the FCC lattice

Moriya [3,4] has developed a microscopic model for calculating the $\mathbf{D}_{ij}$ vector which is valid for localized magnetic systems. For simplicity, the calculation is presented here for the case of one 3d electron (or one 3d hole) on each magnetic site but more complex cases can be studied in the same way. We consider two sites i and j , one site being at the surface, the other one in the first layer below the surface. We describe these two sites by a Hubbard-type Hamiltonian:

$$H = H_0^i + H_0^j + T^{ij} + H_{\text{so}}^i + H_{\text{so}}^j; \quad (1)$$

H_0^i describes the states of a 3d electron localized on site i :

$$H_0^i = \sum_{m,\sigma} \varepsilon_{i,m} c_{im\sigma}^\dagger c_{im\sigma} + U \sum_{m\sigma \neq m'\sigma'} n_{im\sigma} n_{im'\sigma'}, \quad (2)$$

where ε_{im} is the atomic energy of one 3d electron in the orbital m ; ε_{im} is site-dependent because the crystalline field is not the same at the surface and in the bulk. U is the Coulomb repulsion which will be considered as site-independent.

T^{ij} describes the hopping between sites i and j :

$$T^{ij} = \sum_{n,m,\sigma} t_{in,jm} (c_{in\sigma}^\dagger c_{jm\sigma} + c_{jm\sigma}^\dagger c_{in\sigma}), \quad (3)$$

where $t_{in,jm}$ is the hopping integral between orbitals n and m on sites i and j , respectively.

H_{so}^i is the spin–orbit interaction on site i :

$$H_{\text{so}}^i = \lambda \mathbf{L}_i \cdot \mathbf{S}_i. \quad (4)$$

By considering the last three terms of the Hamiltonian of Eq. (1) as a perturbation, it is possible to derive the effective interactions between the spins $\mathbf{S}_i$ and $\mathbf{S}_j$ of the two sites:

$$H_{\text{eff}} = -J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \mathbf{D}_{ij} \cdot (\mathbf{S}_i \times \mathbf{S}_j) + \mathbf{S}_i \mathbf{\Gamma}_{ij} \mathbf{S}_j. \quad (5)$$

The isotropic superexchange interaction J_{ij} is obtained in second order perturbation theory on the Hamiltonian $H_0^i + H_0^j + T^{ij}$: it is of the order of $(t_{ij})^2/U$. The AEI arises in the next order taking into account the spin–orbit coupling: the vector $\mathbf{D}_{ij}$ is found to be proportional to $\lambda(t_{ij})^2/U\Delta$ (Δ being an energy difference between two atomic levels which will be specified in the following). Moriya [3,4] also calculated an anisotropic exchange interaction, $\mathbf{\Gamma}_{ij}$ which is obtained in fourth order of perturbation, this interaction being proportional to $\lambda^2(t_{ij})^2/U\Delta^2$. This last term will not be discussed in this paper. An order of magnitude of these interactions can be derived from the shift Δg of the gyromagnetic ratio, g : $|\mathbf{D}|/J \approx \Delta g/g$, $|\mathbf{\Gamma}|/J \approx (\Delta g/g)^2$, where $\Delta g/g$ is usually not larger than 0.1.

The expression of $\mathbf{D}_{ij}$ will be presented for the (0 0 1) surface of an FCC lattice. The calculation was done following Moriya's scheme with the Hamiltonian of Eq. (1) for the case of one electron in t_{2g} orbitals. To perform the calculation we have to make an assumption on the crystal field energies

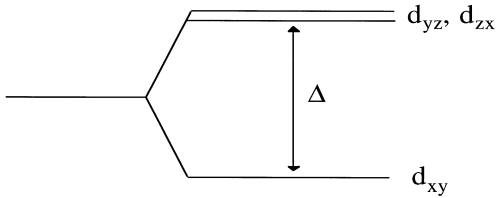


Fig. 1. Crystal field levels on a surface site.

at the surface and in the first layer below the surface. We assume that on a surface site the crystal field splitting is large and the 3d electron occupies the d_{xy} orbital (the x - and y -axes being parallel to the surface, while the z -axis will be taken perpendicular to the surface). The e_g states are supposed to be higher in energy and do not contribute (Fig. 1): the energy splitting Δ is a

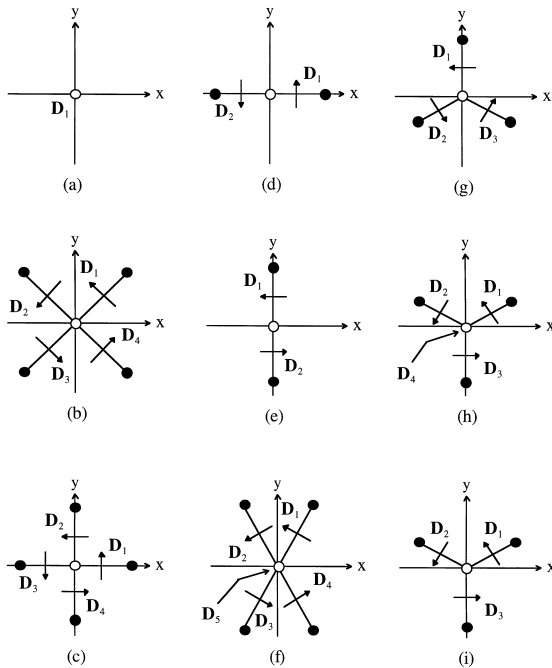


Fig. 2. Projection on the surface plane of the nearest neighbour sites of a surface site for the 9 cases studied in the paper. For each case the choice of x and y axis are indicated. The D_{ij} vectors are shown when they are parallel to the surface plane. When it is not shown, it is perpendicular to the surface. (a), (b) and (c): (0 0 1) surface of the simple cubic, BCC and FCC structures, respectively; (d), (e) and (f): the same for (1 0 1) surface; (g), (h) and (i): the same for (1 1 1) surface plane.

consequence of the symmetry lowering near the surface. Thus it is expected to be much larger at the surface (Δ) than in the first layer (Δ'). In fact, we have considered two different cases: (i) no crystal field splitting in the bulk, i.e. $\Delta' = 0$; (ii) a non-zero crystal field in the first layer, $\Delta' \ll \Delta$, but still large enough to perform a perturbation calculation, i.e. $\Delta' \gg \lambda$ and t_{ij} .

The hopping integrals between a surface site and a neighbouring site below the surface can be calculated for different nearest neighbours. It is found that only the hopping integrals $t_{i,xy;j,xy}$, $t_{i,xy;j,xz}$ and $t_{i,xy;j,yz}$ contribute to D_{ij} : $t_{i,xy;j,xy} = \frac{1}{2}(dd\pi + dd\delta)$ for all i and j sites in neighbouring (0 0 1) planes, while $t_{i,xy;j,xz}$ and $t_{i,xy;j,yz}$ are equal to $\pm \frac{1}{2}(dd\pi - dd\delta)$. ($dd\pi$ and $dd\delta$ are the two-center integrals using the notation introduced by Slater and Koster [14]).

The results are the following: each surface site has four neighbours in the first layer below the surface (Fig. 2c) and the four D_{ij} vectors are parallel to the surface:

$$D_1 = Dy, \quad D_2 = -Dx, \quad D_3 = -Dy, \quad D_4 = Dx. \quad (6)$$

In case (ii) (i.e. $\Delta \gg \Delta' \gg \lambda$ and t_{ij}) we have $D = (\lambda/U)((dd\pi)^2 - (dd\delta)^2)((1/\Delta) - (1/\Delta'))$. If $\Delta' = 0$ (case (i)), we find: $D \approx (\lambda/U)((dd\pi)^2 - (dd\delta)^2)(1/\Delta)$ since the spin-orbit interaction on the bulk site gives a much smaller contribution (of the order of $\lambda^2 U/t_{ij}^2$) because the three t_{2g} orbitals are equally occupied. Calculation for intermediate values of Δ' are not easy within this formalism.

In this model AEI arises since the crystal field splitting is different at the surface and in the first layer below the surface. Moreover, as shown in the next section, the results [Eq. (6)] are consistent with the symmetry considerations developed by Dzyaloshinsky [1,2].

2.2. AEI due to 3-sites mechanism: (0 0 1), (1 0 1) and (1 1 1) surfaces of a simple cubic structure

Another mechanism for AEI was proposed by Levy and Fert [15]: this mechanism involves a 3-sites interaction, two magnetic sites and one non-magnetic site on which spin-orbit interaction occurs, while Moriya's interaction is a 2-sites

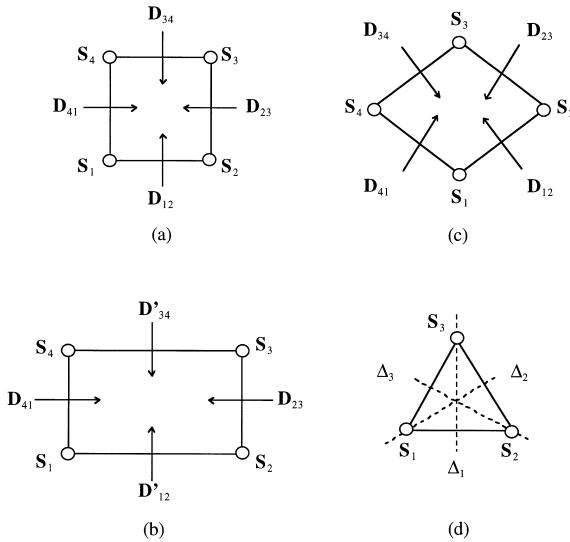


Fig. 3. $\mathbf{D}_{ij}$ vectors for two surface sites. (a): cases a, b, c of Table 2; (b): cases d and f of Table 2; (c): case e; $\mathbf{D}_{ij}$ is in the surface plane, but the angle between $\mathbf{D}_{ij}$ and $\mathbf{R}_{ij}$ is not determined. (d): cases g, h, i; $\mathbf{D}_{ij}$ is in a plane perpendicular to $\mathbf{R}_{ij}$ (indicated by Δ_1 , Δ_2 and Δ_3).

interaction, with spin–orbit coupling on the magnetic sites. Both mechanisms are expected to be important in different situations: the 2-sites mechanism applies to rather localized magnetic systems, while the 3-sites mechanism involves the conduction band and is more appropriate to itinerant systems. Moreover the 3-sites mechanism may give rise to AEI between two surface sites as shown in Ref. [13], while the 2-sites mechanism requires a different crystal field splitting for the 2 sites and vanishes between two surface sites in all cases considered in this paper.

We have calculated the AEI due to 3-sites mechanism for a cubic crystal: the magnetic atoms are supposed to form a simple cubic lattice while the non-magnetic atoms responsible for spin–orbit coupling are in the center of the cube (i.e. CsCl structure). Then the expression derived by Levy and Fert in Ref. [15] yields the following expression for the interaction between two magnetic sites:

$$\mathbf{D}_{ij} = \frac{D_0}{R_{ij}} \sum_n \frac{\mathbf{R}_{in} \cdot \mathbf{R}_{jn} (\mathbf{R}_{in} \times \mathbf{R}_{jn})}{(R_{in} R_{jn})^3}, \quad (7)$$

where $\mathbf{R}_{in}(\mathbf{R}_{jn})$ is the vector joining the magnetic site $i(j)$ to the non-magnetic site n . D_0 is proportional to the spin–orbit coupling and measures the strength of the interaction; in Ref. [15] it was shown that $D_{ij}/J_{ij} \approx \lambda \rho(E_F)$ implying that the calculation is valid for $\lambda \rho(E_F) \ll 1$. For the cubic system considered in this section, we calculate the leading contribution to $\mathbf{D}_{ij}$ for nearest neighbours surface sites using Eq. (7), and considering only nearest neighbours non-magnetic sites (n).

- (0 0 1) surface: AEI occurs between nearest neighbours sites at the surface, two non-magnetic atoms below the surface should be considered for each pair (ij); $\mathbf{D}_{ij}$ is perpendicular to $\mathbf{R}_{ij}$ and in the surface plane (Fig. 3a).
- (1 0 1) surface: as in the preceding case, AEI occurs between neighbouring surface sites with $\mathbf{D}_{ij}$ perpendicular to $\mathbf{R}_{ij}$ and in the surface plane (Fig. 3b); for this case there are in principle three non-magnetic atoms to consider in Eq. (7): two of them are in the surface plane and give a vanishing contribution since they do not break the symmetry, and only one below the surface contributes to AEI.
- (1 1 1) surface: in this case, Eq. (7) leads to AEI between a surface site and a site below the surface (similar to what is obtained from the Moriya's mechanism) and to AEI between surface sites, both of the same order of magnitude. For two surface sites, only one non-magnetic site n below the surface is involved in the mechanism and $\mathbf{D}_{ij}$ is perpendicular to the triangle (ijn): thus it is perpendicular to $\mathbf{R}_{ij}$ but not in the surface plane (Fig. 3d).

Thus we have described two mechanisms which can be responsible for AEI at the surface. In the next section we show that the direction of $\mathbf{D}_{ij}$ can be determined for most surfaces using symmetry arguments, but the strength of the coupling depends on the mechanism involved in the interaction.

2.3. Other surfaces: determination of $\mathbf{D}_{ij}$ by symmetry arguments

Dzyaloshinsky [1,2] has shown that the direction of the vector $\mathbf{D}_{ij}$ obeys the following rules:

Table 1

Direction of the $\mathbf{D}_{ij}$ vectors for nearest neighbours sites at the surface and in the bulk in cubic structures. The z axis is always perpendicular to the surface and x and y axes are in the surface plane (see Fig. 2 for the definition of these axes and the position of the different sites). D refers to sites in the 1st layer and D' to sites in the 2nd (or 3rd) layer below the surface

	(0 0 1) surface	(1 0 1) surface	(1 1 1) surface
Simple cubic lattice	(a) 1 neighbour in 1st layer $\mathbf{D}_1 = D\mathbf{z}$	(d) 2 neighbours in 1st layer $\mathbf{D}_1 = D\mathbf{y}$ $\mathbf{D}_2 = -D\mathbf{y}$	(g) 3 neighbours in 1st layer $\mathbf{D}_1 = -D\mathbf{x}$ $\mathbf{D}_2 = D(\frac{1}{2}\mathbf{x} - \frac{1}{2}\sqrt{3}\mathbf{y})$ $\mathbf{D}_3 = D(\frac{1}{2}\mathbf{x} + \frac{1}{2}\sqrt{3}\mathbf{y})$
BCC lattice	(b) 4 neighbours in 1st layer $\mathbf{D}_1 = D(-\mathbf{x} + \mathbf{y})$ $\mathbf{D}_2 = D(-\mathbf{x} - \mathbf{y})$ $\mathbf{D}_3 = D(\mathbf{x} - \mathbf{y})$ $\mathbf{D}_4 = D(\mathbf{x} + \mathbf{y})$	(e) 2 neighbours in 1st layer $\mathbf{D}_1 = -D\mathbf{x}$ $\mathbf{D}_2 = D\mathbf{x}$	(h) 3 neighbours in 1st layer 1 in 3rd layer $\mathbf{D}_1 = D(-\frac{1}{2}\mathbf{x} + \frac{1}{2}\sqrt{3}\mathbf{y})$ $\mathbf{D}_2 = D(-\frac{1}{2}\mathbf{x} - \frac{1}{2}\sqrt{3}\mathbf{y})$ $\mathbf{D}_3 = D\mathbf{x}$ $\mathbf{D}_4 = D'\mathbf{z}$
FCC lattice	(c) 4 neighbours in the 1st layer $\mathbf{D}_1 = D\mathbf{y}$ $\mathbf{D}_2 = -D\mathbf{x}$ $\mathbf{D}_3 = -D\mathbf{y}$ $\mathbf{D}_4 = D\mathbf{x}$	(f) 4 neighbours in the 1st layer, 1 in 2nd layer $\mathbf{D}_1 = D(-\frac{\sqrt{2}}{3}\mathbf{x} + \frac{1}{\sqrt{3}}\mathbf{y})$ $\mathbf{D}_2 = D(-\frac{\sqrt{2}}{3}\mathbf{x} - \frac{1}{\sqrt{3}}\mathbf{y})$ $\mathbf{D}_3 = D(-\frac{\sqrt{2}}{3}\mathbf{x} - \frac{1}{\sqrt{3}}\mathbf{y})$ $\mathbf{D}_4 = D(-\frac{\sqrt{2}}{3}\mathbf{x} + \frac{1}{\sqrt{3}}\mathbf{y})$ $\mathbf{D}_5 = D'\mathbf{z}$	(i) 3 neighbours in 1st layer $\mathbf{D}_1 = D(-\frac{1}{2}\mathbf{x} + \frac{1}{2}\sqrt{3}\mathbf{y})$ $\mathbf{D}_2 = D(-\frac{1}{2}\mathbf{x} - \frac{1}{2}\sqrt{3}\mathbf{y})$ $\mathbf{D}_3 = D\mathbf{x}$

Table 2

Direction of the $\mathbf{D}_{ij}$ vectors for nearest neighbours surface sites in cubic structures. The z axis is always perpendicular to the surface and x and y axes are in the surface plane (see Fig. 3 for the definition of these axes and the position of the different sites). For each case the two-dimensional structure of the surface sites is indicated

	(0 0 1) surface	(1 0 1) surface	(1 1 1) surface
Simple cubic lattice	(a) Square lattice $\mathbf{D}_{12} = D\mathbf{y}$ $\mathbf{D}_{23} = -D\mathbf{x}$ $\mathbf{D}_{34} = -D\mathbf{y}$ $\mathbf{D}_{41} = D\mathbf{x}$	(d) Rectangular lattice $\mathbf{D}_{12} = D'\mathbf{y}$ $\mathbf{D}_{23} = -D\mathbf{x}$ $\mathbf{D}_{34} = -D'\mathbf{y}$ $\mathbf{D}_{41} = D\mathbf{x}$	
BCC lattice	(b) Square lattice $\mathbf{D}_{12} = D\mathbf{y}$ $\mathbf{D}_{23} = -D\mathbf{x}$ $\mathbf{D}_{34} = -D\mathbf{y}$ $\mathbf{D}_{41} = D\mathbf{x}$	(e) 'lozenge' lattice $\mathbf{D}_{ij}$ in the surface plane, direction is not determined (Fig. 3c)	(g), (h) and (i) direction of $\mathbf{D}_{ij}$ is not completely determined. (see Fig. 3d)
FCC lattice	(c) Square lattice $\mathbf{D}_{12} = D(-\mathbf{x} + \mathbf{y})$ $\mathbf{D}_{23} = D(-\mathbf{x} - \mathbf{y})$ $\mathbf{D}_{34} = D(\mathbf{x} - \mathbf{y})$ $\mathbf{D}_{41} = D(\mathbf{x} + \mathbf{y})$	(f) Rectangular lattice $\mathbf{D}_{12} = D'\mathbf{y}$ $\mathbf{D}_{23} = -D\mathbf{x}$ $\mathbf{D}_{34} = -D'\mathbf{y}$ $\mathbf{D}_{41} = D\mathbf{x}$	

(i) When a center of inversion is located on site M , in the middle of sites 1 and 2, $\mathbf{D}_{ij} = 0$; (ii) if there is a mirror plane perpendicular to $\mathbf{R}_{12} = \mathbf{R}_1 - \mathbf{R}_2$ and passing through site M , $\mathbf{D}_{ij}$ is parallel to this plane; (iii) if there is a mirror plane containing both sites 1 and 2, $\mathbf{D}_{ij}$ is perpendicular to this plane; (iv) when a twofold rotation axis perpendicular to $\mathbf{R}_{12}$ passes through M , $\mathbf{D}_{ij}$ is perpendicular to this axis; (v) if there is an n -fold axis ($n \geq 2$) along $\mathbf{R}_{12}$, $\mathbf{D}_{ij}$ is parallel to $\mathbf{R}_{12}$.

Using these rules it is possible to find the direction of $\mathbf{D}_{ij}$ between one site at the surface and one site below the surface or between two surface sites for a given surface. Some examples for nearest neighbour interactions in cubic structures are given in Tables 1 and 2. Figs. 2 and 3 indicate the directions of the $\mathbf{D}_{ij}$ for the same cases as in Tables 1 and 2.

(i) *AEI between surface and bulk sites* (Table 1 and Fig. 2). In cases (f) and (h) there are nearest neighbours in the first and second (or third) layers below the surface, with different AEI, D and D' . In cases (b)–(e), (g) and (i) all $\mathbf{D}_{ij}$ vectors are parallel to the surface and the sum $\mathbf{D}_i = \sum_j \mathbf{D}_{ij}$ vanishes, while in cases (a), (f) and (h) this sum does not vanish because one of the $\mathbf{D}_{ij}$ is perpendicular to the surface. As will be shown in Section 3 the effect of AEI is different when $\mathbf{D}_i = \sum_j \mathbf{D}_{ij}$ is equal to zero (type A) or different from zero and perpendicular to the surface (type B).

(ii) *AEI between two surface sites* (Table 2 and Fig. 3). In this case, the Dzyaloshinsky rules [1,2] are not always sufficient to determine $\mathbf{D}_{ij}$: in cases (a)–(f) $\mathbf{D}_{ij}$ is in the surface plane and perpendicular to $\mathbf{R}_{ij}$ but in some cases (e), (g), (h) and (i) the direction of $\mathbf{D}_{ij}$ is not completely determined and it should be determined from a microscopic model; e.g. we have shown above that in case (g) Eq. (7) determines the direction of $\mathbf{D}_{ij}$ for a given distribution of the non-magnetic sites (Section 2.2).

Thus these calculations show that AEI may be different from zero near a surface. Several factors influence this interaction: the character of the occupied orbitals and the crystal field scheme, the crystal structure, the direction of the surface, the number of 3d electrons. Also deformations of the lattice, which often occur near a surface or inter-

face, may give rise to AEI. Each experimental case is different and realistic calculations of D can be made in each case, taking into account all these parameters.

3. Modifications of the magnetic ordering near the surface due to the AEI between a surface and a bulk site

In the preceding section it was shown that AEI exists between surface and bulk sites due to a different environment. In this section it will be shown that this interaction modifies the magnetic structure near the surface. We consider one example of each type A and B: for type A we study the (0 0 1) surface of an FCC lattice and for type B, the (1 1 1) surface of a BCC structure. However the results can be generalized easily to other surfaces depending on the classification given in Section 2.3.

3.1. FCC structure with a (0 0 1) surface (type A)

For this surface we have $\mathbf{D}_i = \sum_j \mathbf{D}_{ij} = 0$ for all surface sites i . Thus, from Eq. (6) it can be seen that the AEI will not play any role if the system is ferromagnetic: the four neighbours of the surface atom are in the same layer and it is then natural to suppose that their magnetic moments are the same if the system is ferromagnetic: $\mathbf{S}_1 = \mathbf{S}_2 = \mathbf{S}_3 = \mathbf{S}_4$. Then the interaction energy of the surface atom, characterized by $\mathbf{S}_s$, with its four neighbours of the 1st layer, $E_s = (\sum_{i=1}^4 \mathbf{D}_{is} \cdot \mathbf{S}_i) \times \mathbf{S}_s$, vanishes and there is no modification of the ferromagnetic ordering.

However, the AEI may have some influence if the ground state is antiferromagnetic. In fact in the FCC structure several (degenerate if only nearest neighbour exchange J_1 is considered) antiferromagnetic orderings exist. A negative second neighbour interaction stabilizes the type II antiferromagnetic structure (alternating ferromagnetic (1 1 1) planes). With AEI this structure is changed into a four sublattice structure: in each of the ferromagnetic (1 1 1) plane, two sublattices are formed with a small angle between the spins (of the order of D/J). The resulting structure is a four-sublattice one

and weak ferromagnetism is stabilized with a small magnetization proportional to D/J and parallel to the surface plane.

The same result is obtained for all type A surfaces: no effect is expected for ferromagnets, at least for small values of D/J , while for antiferromagnets weak ferromagnetism may exist. The effect also depends on the easy axis direction: the energy due to AEI is appreciable only for perpendicular anisotropy since in type A surfaces the $\mathbf{D}_{ij}$ are parallel to the surface. Thus in this case AEI favors perpendicular surface anisotropy.

3.2. BCC structure with a (1 1 1) surface (type B)

For type B surfaces, as $\mathbf{D}_i = \sum_j \mathbf{D}_{ij}$ does not vanish, AEI is expected to play a role, not only in antiferromagnetic materials, but also in ferromagnets. We study one example of such a type B surface, namely the (1 1 1) surface in BCC structure. As indicated in Table 1 and Fig. 2h, a surface atom has one neighbour in 3d layer (numbered as 4 in the following) and three in the 1st layer (numbered as 1, 2 and 3), and the $\mathbf{D}_{ij}$ are expressed as (there are no nearest neighbours in 2nd layer):

$$\begin{aligned} \mathbf{D}_1 &= D(-\tfrac{1}{2}\mathbf{x} + \tfrac{1}{2}\sqrt{3}\mathbf{y}), \\ \mathbf{D}_2 &= D(-\tfrac{1}{2}\mathbf{x} - \tfrac{1}{2}\sqrt{3}\mathbf{y}), \\ \mathbf{D}_3 &= D\mathbf{x}, \quad \mathbf{D}_4 = D'\mathbf{z}. \end{aligned} \quad (8)$$

We consider a ferromagnetic film of n atomic layers and we suppose that the moments of all atoms of a given layer are equal: we call $\mathbf{S}_k$ the moment of the layer k ($1 \leq k \leq n$). Since $\mathbf{D}_1 + \mathbf{D}_2 + \mathbf{D}_3 = 0$ there is no effect of AEI between the surface and the first layer, but only between the surface ($k = 1$) and the 3d layer below the surface ($k = 4$) and, for the n -layers film, between $k = n$ and $k = n - 3$ layers. Assuming a nearest neighbour exchange interaction $J > 0$, the total magnetic energy for the film is given by

$$E = ND'\mathbf{z} \cdot [\mathbf{S}_1 \times \mathbf{S}_4 + \mathbf{S}_n \times \mathbf{S}_{n-3}] - NJ \left[3 \sum_{k=1}^{n-1} \mathbf{S}_k \cdot \mathbf{S}_{k+1} + \sum_{k=1}^{n-3} \mathbf{S}_k \cdot \mathbf{S}_{k+3} \right] + nE_L, \quad (9)$$

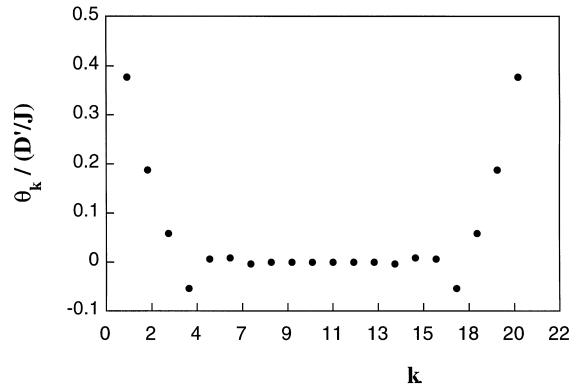


Fig. 4. Deviation angle θ_k as a function of k for $n = 20$ (see text in Section 3.2).

where E_L is the exchange between moments belonging to the same ferromagnetic layer, N is the number of sites of one layer. In the present case there are no nearest neighbours in the same layer and $E_L = 0$. In the general case, E_L does not depend on the canting of the structure (since it is supposed that in each layer the moments remain aligned) and this last term does not play any role in the calculation.

The ferromagnetic state of the film has an energy $E_0 = -2JN(2n - 3)S^2$. The effect of AEI depends on the easy magnetisation axis direction: if the easy axis is perpendicular to the surface, the AEI does not modify the ferromagnetic structure of the film. But if there is an easy axis in the surface plane the ferromagnetic state is modified: e.g., for an easy axis along the x -direction the results obtained by minimizing the energy of Eq. (9), are the following: the moments stay parallel to the surface but deviations from the x -direction occur in all the layers of the film. Fig. 4 shows the deviation angle θ_k of the k th layer for a film of 20 layers: θ_k oscillates with k but only the first oscillation is large; deviations occur in the first 4 planes. Fig. 5 shows the ratio of the two components of the total magnetisation: M_y/M_x ; this ratio increases linearly with D'/J and the slope is larger for smaller values of n .

The same results are obtained for the other type B surfaces: for in-plane anisotropy, deviations of the spin directions are obtained, and this leads to a rotation of the total magnetisation which can be of the order of a few degrees for typical values of $D'/J \approx 0.1$.

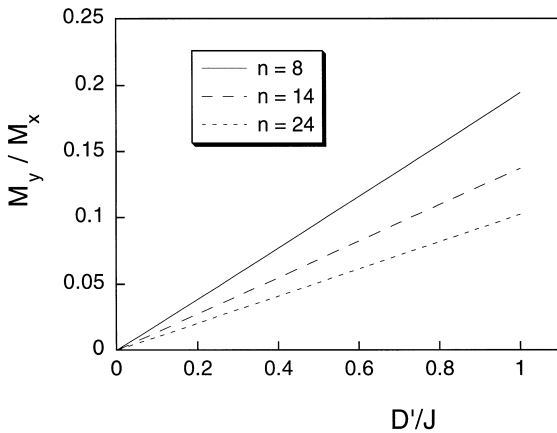


Fig. 5. Ratio M_y/M_x as a function of D'/J for several values of n .

4. Modifications of the magnetic ordering near the surface due to the AEI between two surface sites

In this section we show that AEI between surface sites can be responsible for a rearrangement of the surface structure and can give contribution to the surface anisotropy. We consider the case of a ferromagnetic simple cubic thin film with (0 0 1) surfaces and AEI at both surface planes. In the central layer the spins are aligned in the same direction and only the surface spins are allowed to rotate. We have considered three different directions for the central layer's spins, corresponding to different easy anisotropy axis in the bulk; in each case the surface spins are slightly tilted, forming a four sublattice structure:

(i) The central layer's spins are perpendicular to the film. Minimization of the total energy leads to canting angles equal to $\sqrt{2D/3J}$ with respect to the z axis. The energy gain per surface site is then: $\Delta E = -\frac{2}{9}(D/J)^2JS^2$;

(ii) The central layer's spins are in the film plane, parallel to the x axis. At the surface the spins are making a small angle with the surface (equal to $D/3J$) and the energy gain per surface site is: $\Delta E = -\frac{1}{9}(D/J)^2JS^2$. The same energy is obtained if the spins are parallel to the (1 1 0) axis (but the values of the canting angles are different).

In all cases the resulting magnetization is reduced at the surface due to the canting of the

magnetic moments, but the direction of the total magnetization is not changed. Moreover the energy gain depends on the direction of the magnetization: in the present case ((1 0 0) surface of a simple cubic lattice) perpendicular anisotropy is favoured because the D_{ij} are in the surface plane. Thus this effect contributes to the surface anisotropy energy.

5. Conclusions

We have shown the AEI is present close to magnetic surfaces or interfaces. In most cases, the symmetry rules determine the direction of D_{ij} . Two different mechanisms have been proposed for calculating the order of magnitude of this interaction. We have made some predictions concerning its consequences on the magnetic structure in magnetic films or multilayers: surface reorientations or weak ferromagnetism may occur. We have shown also that AEI contributes to the surface anisotropy energy since it always favours magnetic structures where the moments are perpendicular to D_{ij} .

We have studied separately AEI between two surface sites and between surface and bulk sites, but in general both types can be present and give rise to more complex rearrangements of the magnetic structure.

AEI may also be present at interfaces in bilayers or multilayers: recently it was shown that in a three-layers system (two ferromagnetic layers separated by a paramagnetic layer), spin-orbit interaction at interfaces is responsible for AEI between the ferromagnetic layers [16] and this interaction induces a non-collinear interlayer coupling.

Finally, it can be pointed out that AEI may have consequences not only on the magnetic arrangement but also on other properties: e.g., it was shown that new magneto-electric effects arise in multilayers with antisymmetric exchange interactions [17].

Acknowledgements

We thank A. Fert for a critical reading of the manuscript and several interesting suggestions.

References

- [1] I. Dzyaloshinsky, *Sov. Phys. JETP* 5 (1957) 1259.
- [2] I. Dzyaloshinsky, *J. Phys. Chem. Solids* 4 (1958) 241.
- [3] T. Moriya, *Phys. Rev. Lett.* 4 (1960) 228.
- [4] T. Moriya, *Phys. Rev.* 120 (1960) 91.
- [5] P.W. Anderson, *Phys. Rev.* 115 (1959) 2.
- [6] T. Thio, T.R. Thurston, N.W. Preyer, P.J. Picone, M.A. Kastner, H.P. Jenssen, D.R. Gabbe, C.Y. Chen, R.J. Birgeneau, A. Aharony, *Phys. Rev. B* 38 (1988) 905.
- [7] D. Coffey, T.M. Rice, F.C. Zhang, *Phys. Rev. B* 44 (1991) 10112.
- [8] L. Shekhtman, O. Entin-Wohlman, A. Aharony, *Phys. Rev. Lett.* 69 (1992) 836.
- [9] N.E. Bonesteel, *Phys. Rev. B* 47 (1993) 11302.
- [10] A. Rouco, X. Obradors, M. Tovar, F. Perez, D. Chateigner, P. Bordet, *Phys. Rev. B* 50 (1994) 9924.
- [11] D.A. Smith, *J. Magn. Magn. Mater.* 1 (1976) 214.
- [12] A. Fert, P.M. Levy, *Phys. Rev. Lett.* 44 (1980) 1538.
- [13] A. Fert, in: A. Chamberod, J. Hillairat (Eds.), *Materials Science Forum*, vol. 59–60, 1990, p. 444.
- [14] J.C. Slater, G.F. Koster, *Phys. Rev.* 94 (1954) 1498.
- [15] P.M. Levy, A. Fert, *Phys. Rev. B* 23 (1981) 4667.
- [16] K. Xia, W. Zhang, M. Lu, H. Zhai, *Phys. Rev. B* 55 (1997) 12561.
- [17] E.A. Turov, *Europhys. Lett.* 34 (1996) 305.